Data assimilation diagnostics: Assessing the impact of observations on the forecast

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Data Assimilation Training Course, 7 March 2024

Acknowledgements to: <u>Cristina Lupu</u>, <u>Alan Geer</u>, N. Bormann, T. McNally, M. Dahoui, S. Healy, L. Isaksen and C. Cardinali



Overview

- What, why, how?
- Main observing systems (for global NWP)
- Observing System Experiments OSEs
 - What do we verify against?
- Adjoint-based diagnostic methods Forecast Sensitivity to Observation Impact
- Examples: factors affecting impact/FSOI
- Other methods not covered here (EFSOI, EDA spread, OSSE)
- Summary

An aircraft problem (found Dec 2023)

- Affects a subset (B787) of Chinese and US AMDARS wrong sign of latitude!!
- <u>https://www.ecmwf.int/en/forecasts/quality-our-forecasts/monitoring-observing-system</u>
- O-A less noisy than O-B useful to highlight the issue ⁽²⁾

150°W

120°W

90°W

60°W

30°W

0°E

30°E

60°E



-0.14

30°E

60° F

90°E

120°E

150°E

120°E

90° E

150°E

-0.36

What are the questions?

- For a given subset of observations (eg aircraft winds):
- Do they improve the forecast? How much?
- How do we measure improvement? Need metric and 'the truth'.
- What factors influence the impact? (observation density, synoptic variability, ..)
 - Answers depend on the DA system, and all the other observations
- Planning observation networks ...
- What, where, how frequent, how high,
- Or NMS is considering shutting a radiosonde station 'how important is it?'

The Global Observing System Network

 ECMWF makes use of wide variety of conventional and satellite observations. The 4D-Var data assimilation system is assimilating ~10⁷ observations per a 12-h assimilation window;



- Conventional observations Surface (land/marine) Aircraft Radiosonde
 - Satellite observations Infrared (IR) and Microwave (MW) radiances from LEO and GEO satellites Atmospheric Motion Vectors (AMVs) GPS Radio occultation Scatterometer Aeolus Horizontal Line-of-sight winds Other (ozone, etc)

 Information on the quality/availability of the different components of the observing system used/monitored by ECMWF: <u>https://www.ecmwf.int/en/forecasts/quality-our-forecasts/monitoring-observing-system</u>

Data sources : in situ ('conventional') observations

- Directly measure the required meteorological variables such as temperature, humidity, ...
- Limited in spatial/temporal coverage;



Instrument

Parameters



SYNOP-SHIP- METAR	<u>MSL pressure,</u> 10-m wind, 2m-rel humidity, temperature
BUOY	Wind, temperature, <u>MSL pressure</u>
TEMP TEMPSHIP DROPSONDES	Wind, temperature, spec. humidity
PROFILER	Wind
PILOT	Wind
AIRCRAFT	Wind, temperature, spec. humidity





	spec. humidity
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Data sources: Satellite observations

- Provide indirect measurements of the atmospheric state;
- Frequent and spatially detailed measurements over the entire globe;
 - Geostationary satellites (GEO): ~36000 km altitude provide near-continuous views of a fixed geographical area;
 - Satellites in Low Earth Orbit (LEO): ~1000km provide near-global coverage in 12h, but only return to the same location typically twice by day (more frequent at high latitudes);



Satellite observations used

System	Variables, Advantages	Caveats, Notes
Microwave (MW) & Infrared (IR) sounders	Temperature, humidity, SST Near-global MW sees through ice cloud but senses water cloud, rain and snow	Limited vertical resolution IR blocked by cloud Needs Bias Correction (BC) Difficult to use over ice/snow
Motion vectors (AMVs)	Wind, quasi-global	Coverage gaps, height assignment issues
Radio occultation	Hi-Res refractivity, No bias corr.	Gives T at upper levels, humidity at lower levels
Scatterometer	Ocean surface winds	Directional ambiguity
Doppler wind lidar	Line-of-sight winds	Prototype needs BC
MW imagers	Integrated water vapour, cloud and rain, surface winds, sea ice	Used over the ocean, limited use over land; sea ice in development
Ozone	Ozone	Limited vertical resolution

In situ observations

System	Variables, Advantages	Caveats, Notes
Aircraft	Wind, temperature, some humidity Locally high density Low cost	Very uneven distribution T needs bias correction (BC)
Radiosondes	Wind, temperature, humidity High vertical resolution Closest to reference obs	Low density + gaps Humidity quality mixed in upper troposphere
Surface	Pressure, temperature, humidity, wind, SST, snow depth Locally high density	Sparse over oceans/deserts Some representation issues
GroundGPS	Integrated water vapour	Problems with profile of increments near BL top? To be used at ECMWF from cycle 49r1.

Adapted and updated from Ingleby et al (2021)



With millions of observations assimilated every analysis cycle, how do we quantify the value provided by all these data?

Proportion of assimilated observations (Total number: ~ 33 Million per 24 h)



ops 1-Jan-2022 to 31-Dec-2022

What diagnostics are available to measure impact?

Which observation types provide the largest total impacts, or largest impact per observation?

How do impacts vary by location or channel?

Do all observations provide benefit?

Observing system experiments

A simple scalar example where analysis error = 1/sqrt(1+number of observations) Impact of observations is **context dependent**



Observing System Experiments (OSEs)



- Requires re-running the data assimilation system for each subset of observations examined. Costly, because of the length of time required to get statistically significant results (Geer, 2016)
- Medium-range forecasts have been run from NO SAT and NO CONV experiments and their quality evaluated by comparison to CTRL.
 - Both denial experiments produce forecast errors larger than those of the CTRL, but the denial of all satellite observations results in a significantly larger degradation of quality than the denial of conventional observations.
- Valid for any forecast range or measure:
 - Range (12-h, 5 days, 10 days...)
 - Parameter (geopotential height, temperature, wind, humidity...)
 - Altitude (surface, 500hPa, 1hPa)
 - Region (global, NH, SH, Tropics., ...)

OSEs for main observing systems

- OSEs are performed regularly at ECMWF (e.g., Bormann *et al.*, 2019; McNally, 2014; Radnoti *et al.*, 2010; Kelly *et al.*, 2004), but because of their expense usually involve a limited number of experiments, each considering relatively large subsets of observations.
- Assess and understand the relative contribution of each component of the observing network to the overall health of the forecasting system because:
 - The impact of observations may change over time depending on the model / DA evolution and the availability of new data
 - Important to explore resilience and redundancy to optimise the use of resources
 - Useful for the long term planning of the global observing system



- Denial experiments compared to a full system for (Bormann et al., 2019): All conventional observations MW radiances IR sounder radiances AMVs GPSRO
 - Periods: 1 June – 30 September 2016; 1 December 2017 – 31 March 2018;

Current impact of various observing systems: Z 500 hPa

Conventional observations and microwave radiances are the main drivers of headline scores in the ECMWF system, with infrared sounders adding further robustness for a wide range of geophysical variables (see, Bormann et al., 2019)



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Periods: 1 June – 30 September 2016; 1 December 2017 – 31 March 2018;

Current impact of various observing systems: Wind at 850 hPa



- The results confirm the complementarity of the global observing system:
 - Atmospheric Motion Vectors add benefits for tropospheric wind, particularly in the tropics and at the short range;
 - GPSRO shows significant impact in the upper troposphere/lower stratosphere, particularly temperature.



What is the truth? (for use in verification)

- We want the 'reference' to be
 - Accurate and unbiased
 - Independent
 - Complete (well sampled)
- All alternatives have pros and cons
 - E.g. 'own analysis' is not independent at short-range



Verification vs observations, operational analysis, own analysis), taken from Lawrence et al. (2019).

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Adjoint-based diagnostic methods (FSOI)

- Estimates of observation impact using the adjoint (transpose) of the data assimilation system have become increasingly popular as an alternative/complement to traditional OSEs.
 - Enable a simultaneous estimate of forecast impact for any and all observations assimilated.
 - Impact assessed without denial FSOI measures the impact of observations when the entire observation dataset is present in the assimilation system
 - Doesn't measure the **anchoring** of bias correction by GPSRO and sondes
 - Used at several centers now for routine monitoring or experimentation: ECMWF, Met Office; Meteo France, JMA, NRL, GMAO, Bureau of Meteorology
 - Implemented at ECMWF by C. Cardinali (2009); FSOI statistics are published on the ECMWF monitoring website: <u>https://www.ecmwf.int/en/forecasts/quality-our-forecasts/monitoring-observing-system</u>

Forecast Sensitivity Observation Impact Measure Cardinali (2009), Langland and Baker (2004), <u>Errico (2007)</u>



Observations move the forecast from the background trajectory to trajectory starting from the new analysis;

The difference $\delta e = e(\mathbf{x}_a^f) - e(\mathbf{x}_b^f)$ measures the collective impact at 24-h of **all observations** assimilated at 0-h. (model space)

Can we measure their individual contributions? (observation space) Yes, using information from the model and analysis adjoints.

Forecast error norm

• Define a scalar cost function of the forecast error:

$$\boldsymbol{e} = (\mathbf{x}^f - \mathbf{x}_t)^T \mathbf{C} (\mathbf{x}^f - \mathbf{x}_t)$$

where $\mathbf{x}^{t} = M\mathbf{x}$ is the forecast model state, x_{t} is the truth atmospheric state, M is the nonlinear model and \mathbf{C} - is a matrix of energy norm coefficients. The verifying analysis is a proxy for the truth atmospheric state.

• Energy norm based cost function:

u- is the zonal wind, v is the meridional wind, R_d is the dry air constant, T_r is the reference temperature (350 K), p_r is the reference pressure (1000 hPa) and T is the air temperature, q specific humidity with a certain weight w_q , Lc is the latent heat of condensation, S is horizontal dimensions ECMWF $\rightarrow w_q$ =0 (dry energy norm)

$$\mathbf{x}^{\mathrm{T}}\mathbf{C}\mathbf{x} = \frac{1}{2} \int_{p_0}^{p_1} \iint_{S} (u^2 + v^2 + \frac{c_p}{T_r} T^2 + w_q \frac{L_c^2}{c_p T_r} q^2) dp dS + \frac{1}{2} R_d T_r p_r \int_{S} (\ln p_{sfc})^2 dS$$

- A dry norm based on own-analysis verification is used in the operational FSOI (w_q=0), but a moist energy norm or an observation-based error norm have also been advocated (Janisková and Cardinali, 2016; Cardinali, 2018)
 - Observation-based norm puts more weight on the stratosphere
 - \mathbf{x}_t Truth in practice, and with some issues, we use the analysis from the same DA system



Impact of initial conditions on the forecast

- We have defined a scalar cost function of the forecast error:
- First order sensitivity of the forecast error to a perturbation in the analysis initial conditions is:
- Assuming that forecast perturbations evolve according to the Jacobian/TL forecast model M
- Then the scalar cost function can be differentiated to get



$$e = (\mathbf{x}^f - \mathbf{x}_t)^T \mathbf{C} (\mathbf{x}^f - \mathbf{x}_t)$$

$$\delta e = (\delta \mathbf{x}_a)^T \, \frac{\partial e}{\partial \mathbf{x}_a}$$

For the full Taylor expansion see Errico (2007)

$$\delta \mathbf{x}^f = \mathbf{M} \delta \mathbf{x}_a$$

$$\frac{\partial e}{\partial \mathbf{x}_a} = 2\mathbf{M}^T \mathbf{C} (\mathbf{x}^f - \mathbf{x}_t)$$

The forecast error is mapped onto the initial conditions by the adjoint of the model, providing, for example, regions that are particularly sensitive to forecast error growth.

Observational impact on the analysis

Recall the analysis equation (Daley, 1991):

$$\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{K}(\mathbf{y} - H\mathbf{x}_{b})$$

$$\delta \mathbf{x}_{a} = \mathbf{K}\delta \mathbf{y}$$
(model space) (observation space)
$$\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{K}(\mathbf{y} - H\mathbf{x}_{b})$$

$$\mathbf{x}_{a} = \mathbf{k}\delta \mathbf{y}$$
(model space) (observation space)
$$\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{k}(\mathbf{y} - H\mathbf{x}_{b})$$

$$\mathbf{x}_{a} = \mathbf{k}\delta \mathbf{y}$$
(model space) (observation space)
$$\mathbf{x}_{a} = \mathbf{x}_{a} - \mathbf{x}_{b}$$
is the analysis vector
$$\mathbf{x}_{b} = \mathbf{b}ackground vector$$

$$\mathbf{x}_{b} = \mathbf{b}ackground vec$$

We use the adjoint of K to convert the forecast sensitivity in model space at initial time to observation space

 The sensitivity of the analysis to the observations is: DFS, Cardinali et al. 2004; Lupu et al., 2011; Daescu, 2008; (separate diagnostic ~weight given to the observations)

$$\frac{\partial \mathbf{x}_a}{\partial \mathbf{y}} = \mathbf{K}^T$$

Observation impact in the IFS

e

• We just derived the first order sensitivity of the 24 h dry forecast error norm to the analysis increments, but as a summation over observations

$$\delta e = 2(\delta \mathbf{y})^T \mathbf{K}^T \mathbf{M}^T \mathbf{C} (\mathbf{x}^f - \mathbf{x}_t)$$
Adjoint analysis scheme

 In practice all NWP centres including ECMWF use an approximately 3rd order accurate sensitivity expansion (Langland and Baker, 2004, Cardinali 2009, Errico, 2007)

$$\delta e = (\delta \mathbf{y})^T \mathbf{K}^T \frac{\partial e}{\partial \mathbf{x}_a} = (\delta \mathbf{y})^T \mathbf{K}^T [\mathbf{M}_a^T \mathbf{C}(\mathbf{x}_a^f - \mathbf{x}_t) + \mathbf{M}_b^T \mathbf{C}(\mathbf{x}_b^f - \mathbf{x}_t)]$$
Fest Error
$$e$$

$$e$$

$$e$$

$$M_b^T \mathbf{C}(\mathbf{x}_b^f - \mathbf{x}^t) = e_{36}$$

$$M_b^T \mathbf{C}(\mathbf{x}_a^f - \mathbf{x}^t) = e_{36}$$

$$\int_{a_a} \mathbf{M}_a^T \mathbf{C}(\mathbf{x}_a^f - \mathbf{x}^t)$$

$$\int_{a_a} \mathbf{M}_a^T \mathbf{C}(\mathbf{x}_a^f - \mathbf{x}^t) = e_{36}$$

$$\int_{a_a} \mathbf{M}_a^T \mathbf{C}(\mathbf{x}^f - \mathbf{x}^t) = e_{36}$$

$$\int_{$$

FSOI in the IFS - summary

$$\delta e = (\delta \mathbf{y})^T \mathbf{K}^T \frac{\partial e}{\partial \mathbf{x}_a}$$

- FSOI is a function of sensitivity gradient, the adjoint of the gain matrix and the innovation vector;
- FSOI is computed at ECMWF for a 12-h window; The sensitivity gradient is valid at the starting time of the 4D-Var window, typically 9 UTC and 21UTC;
- The impact of observations can be summed up over time and space in different subsets to compute the total contribution of the different components of the observing system towards reduction of the forecast errors;
- FSOI is influenced by the simplified adjoint model used to carry the forecast error information backwards and by the selection of the total energy norm (dry/moist).
- We found that there are occasional large spikes in the FSOI values :
- Thought to be linked to gravity waves (instabilities)
- For now the few affected dates are removed from the statistics.
- Energy norm emphasises the troposphere





Observation impact calculation

1. Difference of nonlinear forecast error norm (model space)

$$\delta e = e_{24} - e_{36}$$

 $\delta e = (\delta \mathbf{y})^T \frac{\partial e}{\partial \mathbf{y}}$

2. FSOI (observation space) – adjoint-based estimate of δe

 $\delta e < 0$ the observation is beneficial $\delta e > 0$ the observation is non-beneficial FSOI –all observations



Largest FSOI values in the Southern extra-tropics \rightarrow consistent with faster error growth in the winter storm tracks (Geer et al., 2017);

Impact of major observing systems on reducing 24-h forecast errors, January 2020

- Measured using a global dry energy norm, surface to model top
- **Negative** (positive) **FSOI** indicate that the assimilation of an observation or a subset of observations **decreased** (increased) 24-hour forecast error and will be referred as **beneficial** (detrimental).



Examples of Observing System Impacts

• Observation impacts can be sorted by conditional information (e.g. region, separate channels or separate satellites, wind and mass observations, etc)



FSOI of major observing systems in ECMWF operations



All-sky assimilation of humidity sounding channels on SSMIS

assimilation (Geer et al., 2017)



Last 5 years of FSOI

ops 1-Nov-2018 to 30-Nov-2023



FSOI of main data types, April 2023



100% = full operational observing system

Global relative FSOI for conventional obs.

1-Apr-2023 to 30-Apr-2023



- Aircraft give about 10% of total impact;
- Similar to sum of other in situ data: Synop + Sonde + Buoy + Pilot;
- Aeolus Wind lidar (activated since 9 January 2020, lost in May 2023) contributed approximately 3% of the overall reduction in global forecast error;

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Relative FSOI by satellite and instrument (April 2023)



100% = full operational observing system

Impact of individual channels e.g., IASI 39 WV channels



More info on FSOI impact results see references (Geer *et al.*, 2017; Eresmaa *et al.*, 2017; Eresmaa and Lupu, 2017

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What fraction of the assimilated observations improve the forecast ?



• For all data types, only 50-52% of the observations lead to positive impact on the 24-h forecast!

- The numbers of observations that improve or degrade the forecast are both large.
- See Lorenc and Marriott (2014) for more on the "50%" issue

For the analysis we can look at the percentage of values with |O-A| < |O-B| For Jan 2024 in situ data some values were:

- TAMDAR T 59%
- Surface pressure 65-66%
- BUFR radiosonde 68-74%

FSOI depends on observation time in the 4D-Var window

-0.01

-0.02

-0.03

-0.04

-0.05

-0.06

-0.07

-0.08

-0.09





aircraft temperature

aircraft u-wind aircraft v-wind

aircraft humidity

Observations late (4Q) in the 4D-Var window are more influential than data early (1Q) in the window. This is a real

effect - see McNally (2019) OSEs.

Radiosondes at

end of 1Q \otimes



This is because the forecast model can evolve numerous atmospheric variables over time to fit the data at the end of the window.

Observing the Atlantic: AMSU-A MetOp-A versus NOAA-15

Satellite data (in LEO orbit) typically observe the same location at the same local time each day

million km²

x FSOI [J/kg] per

0.0



...at the beginning of the 4D-Var window (MetOp-A)

FSOI no impact over the N. Atlantic



...at the end of the 4D-Var window (NOAA-15)



FSOI-positive impact over the N. Atlantic



Data density

Sondes: FSOI per datum, 2020

Synops: FSOI per datum, 2020





 More impact per station/report from scattered islands in the Pacific

 4 of the radiosondes in the area are maintained by MeteoFrance

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Buoy pressure data

- Biggest impact in Southern Ocean
 data sparse, large (O-B)
- Large impact in NH baroclinic development areas: 'Gulf Stream' and 'Kuroshio'
- Only 60% of drifting buoys have barometer – despite large impact ^(C)
- Ingleby and Isaksen (2018)

SD(O-B) 2014-2016

a)



b) FSOI 2014-2016



c) Rms(Eady index) 2014-2016



Summary of Arctic and Global FSOI





H. Lawrence et al, 2019: Arctic; Global plots unpublished

- 'Conventional' (aircraft, radiosondes, surface) obs mainly occur in NH
- Background errors larger in winter,
- Difficult to use microwave/IR sounders at low levels over ice/snow

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Do OSE and FSOI 'tell the same story'

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- Mostly give similar rankings
- Figure from Eyre (2021) using results from Candy et al (2021) – Met Office
- FSOI: % of impact of all observations
- ODE/DDE: % degradation of T+24 scores when removed (basket of variables/levels)
- Also see presentations from WMO (2020)

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Other ways of estimating observation impact

• Ensemble FSOI (EFSOI)

- An equivalent to FSOI designed for ensemblebased data assimilation systems where the adjoint forecast model is not available – Kalnay et al. (2012)
- EDA spread method
 - Measure the reduction in ensemble spread caused by a perturbation in the observing system
 - Typically used at ECMWF for estimating the impact of future observing systems using simulated data
 - Origin: Harnisch et al. (2013) simulating the impact of many more GNSS observations than currently available
- OSSE Observation system simulation experiment
 - Like an OSE only with simulated observations (e.g. a future sensor)



Closing remarks

- Methods to measure the observation contribution to the forecast quality
 - **OSEs** give definitive answer to the Q: "what if I did not have these observations?"
 - Measures impact at all forecast ranges and enables all aspects of impacts to be assessed in a fully non-linear system and measuring non-localised impact;
 - Extremely expensive to run long periods to achieve statistical significance;
 - FSOI Adjoint-derived observations impact
 - Allows detailed evaluation of observations impact in the current run (e.g., individual channels, different regions or separate satellites); Very affordable (compared to OSE), impact available on a daily basis;
 - The adjoint-based method is restricted by the use of a linearised version of the model, which makes it valid only to evaluate short-range forecasts;
 - The verification state should be ideally uncorrelated with the forecast; this is not the case for 0-48h forecasts when the analysis is used; This apply for any analysis based verification metric for FSOI;
 - FSOI is affected by the optimality of the system use of incorrect B, R, or an inadequate bias correction, for example, will make the results very difficult to interpret (*e.g., Lupu, 2013, 6*th WMO Symposium on Data Assimilation);
 - **FSOI extends, not replace OSEs** (applicable forecast range, metrics differ)

Closing remarks

• Satellite observations, especially radiance data, are critical for global NWP, but conventional data remain very important.

- Observing types with the most significant contributions to error reduction for global NWP: MW sounders, hyperspectral IR sounders, radiosondes, aircraft data and AMVs. On a per observation basis, the impact is dominated by buoys, radiosondes, AMVs and aircraft observations.
- The extension of the use of MW humidity-sounding radiances to all-sky leads to a significant improvement of the forecast impact in the ECMWF system.

• Only a small majority (50-52%) of observations improves the forecast, and most of the overall benefit comes from a large number of observations having small-moderate impacts

- Reliance on statistics of background and observation errors implies a distribution of positive and negative impacts, regardless of data quality.
- Imperfect DA method, errors in the verifying analysis may contribute to the number of observations harming the forecast.

• Observations late in the 4D-Var window are more influential than data early in the window (demonstrated by both OSEs and FSOI)

• Important to ensure that late arriving observations are included in the DA → Continuous data assimilation configuration in IFS since June 2019 (*Lean et al., 2019*)

• Interpretation of forecast improvement or degradation as depicted by the FSOI tool is necessary.

Closing remarks

- Both OSEs and FSOI are used to design/refine elements of the global observing system
 - E.g. relative benefits of wind and temperature observations
 - Observations in data sparse areas have more impact
 - Observations in 'active' areas have more impact
 - FSOI underestimates effect of <u>anchor</u> observations: GPSRO (sondes?)
- Several NWP centres are computing FSOI (Forecast Sensitivity Observation Impact) routinely, although different methodologies are used for different data assimilation systems:
 - adjoint-based FSOI (e.g., ECMWF, Met Office, Meteo France, NRL, GMAO, JMA, Bureau of Meteorology)
 - **ensemble-based** FSOI (e.g., NCEP, JMA)
 - hybrid FSOI for 4DEnVar (e.g, Env. Canada)
- No estimate of the truth is perfect (even ECMWF analysis)!
- Keep asking questions ...

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